Diethyl butanedioate

123-25-1 | DTXSID2038732

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 25.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.81e-01

Confidence level: 5.92e-01

Nearest Neighbors from the Training Set

Image not found
Aldicarb sulfoxide
Measured: 3.63
Predicted: 8.06

Image not found
Aldoxycarb
Measured: 2.63
Predicted: 5.32

Image not found
N-(3-chloro-4-methylphenyl)-N'-methylurea
Measured: 126
Predicted: 99.6

Image not found
Urea, (3-chloro-4-methoxyphenyl)-
Measured: 100
Predicted: 47.5

Image not found
Simazine
Measured: 126
Predicted: 135